UNCLASSIFIED

Defense Technical Information Center Compilation Part Notice

ADP013716

TITLE: Iterative Refinement Schemes for an Ill-Conditioned Transfer Equation in Astrophysics

DISTRIBUTION: Approved for public release, distribution unlimited

This paper is part of the following report:

TITLE: Algorithms For Approximation IV. Proceedings of the 2001 International Symposium

To order the complete compilation report, use: ADA412833

The component part is provided here to allow users access to individually authored sections of proceedings, annals, symposia, etc. However, the component should be considered within the context of the overall compilation report and not as a stand-alone technical report.

The following component part numbers comprise the compilation report:
ADP013708 thru ADP013761

UNCLASSIFIED

Iterative refinement schemes for an ill-conditioned transfer equation in astrophysics

Mario Ahues, Filomena d'Almeida, Alain Largillier, Olivier Titaud and Paulo Vasconcelos

Université de Saint Etienne, France and Universidade do Porto, Portugal

Abstract

Let $X := L^1([0,\tau_0])$, where τ_0 represents the optical depth of a stellar atmosphere. The weakly singular integral operator $T : X \to X$ defined by

$$(T\varphi)(\tau) = \frac{\varpi}{2}\int_0^{\tau_0} E_1(|\tau-\tau'|)\varphi(\tau')\,d\tau',$$

where $\varpi \in]0,1[$ is the albedo of the atmosphere and E_1 denotes the first exponential-integral function, is such that $\|T\|_1 = \varpi(1 - E_2(\tau_0/2))$, where E_2 denotes the second exponential-integral function. If ϖ is close to 1, and τ_0 is large, then $\|T\|_1$ is close to 1. In that case, the *transfer problem*

$$\text{given } f \in X, \text{ find } \varphi \in X \text{ such that } T\varphi = \varphi + f$$

is ill-conditioned, and the convergence of the fixed-point iteration $\varphi_{k+1} = T\varphi_k - f$, which is commonly used by numerical astronomers, becomes prohibitively slow. The purposes of this work are to approximate φ through different sequences whose terms solve well-conditioned approximate equations, and to compare their efficiency and computational costs.

1 Introduction

For a given $\tau_0 > 0$, let g be a function defined on $]0,\tau_0]$ such that

$$\lim_{\tau\to 0^+} g(\tau) = +\infty, \tag{1.1}$$

$$g \in C^0(]0,\tau_0]) \cap L^1([0,\tau_0]), \tag{1.2}$$

$$g(\tau) \geq 0 \text{ for all } \tau \in]0,\tau_0], \tag{1.3}$$

$$g \text{ is a decreasing function on }]0,\tau_0]. \tag{1.4}$$

We consider the integral operator T defined by

$$(Tx)(\tau) := \int_0^{\tau_0} g(|\tau-\tau'|)x(\tau')\,d\tau'. \tag{1.5}$$

Theorem 1 *T is a linear compact operator in $L^1([0,\tau_0])$ and* $\|T\|_1 = 2\int_0^{\tau_0/2} g(\tau)\,d\tau.$

Proof: See [2]. □

For z in the resolvent set of T, we consider the Fredholm equation of the second kind

$$T\varphi = z\varphi + f. \tag{1.6}$$

Applications will concern the function $g :]0, \tau_0] \to I\!R$ given by

$$g(\tau) := \frac{\varpi}{2} E_1(\tau) \tag{1.7}$$

where $\varpi \in]0, 1[$ and E_1 is the exponential-integral function : $E_1(\tau) := \displaystyle\int_1^\infty \frac{\exp(-\tau\mu)}{\mu}\, d\mu$, $\tau > 0$. E_1 is the first function of the sequence $(E_\nu)_{\nu \geq 1}$, $E_\nu(\tau) := \displaystyle\int_1^\infty \frac{\exp(-\tau\mu)}{\mu^\nu}\, d\mu$, $\tau \geq 0$, $\nu \geq 2$, and it is the only one presenting a logarithmic singularity at $\tau = 0$. Following Theorem 1, when g is defined by (1.7), we have $\|T\|_1 = \varpi[1 - E_2(\tau_0/2)] < 1$.

We recall that a bounded linear finite rank operator T_n in a normed linear space X can be written as

$$T_n := \sum_{j=1}^{n} \langle \cdot\,, \ell_{n,j} \rangle e_{n,j} \tag{1.8}$$

where $n \in I\!N^*$, and, for $j \in [\![1, n]\!]$, $\ell_{n,j} \in X^*$, the topological adjoint space of X, and $e_{n,j} \in X$.

The resolution of the approximate equation

$$T_n\varphi_n = z\varphi_n + f, \tag{1.9}$$

where z belongs to the resolvent set of T_n, leads to an n-dimensional linear system

$$(\mathsf{A}_n - z\mathsf{I}_n)\mathsf{x}_n = \mathsf{b}_n \tag{1.10}$$

where I_n is the identity matrix of order n,

$$\mathsf{A}_n(i,j) := \langle e_{n,j}\,, \ell_{n,i} \rangle, \quad \mathsf{b}_n(i) := \langle f\,, \ell_{n,i} \rangle, \quad \mathsf{x}_n(j) := \langle \varphi_n\,, \ell_{n,j} \rangle. \tag{1.11}$$

Once this system is solved, the solution of (1.9) is given by

$$\varphi_n = \frac{1}{z}\left(\sum_{j=1}^{n} \mathsf{x}_n(j) e_{n,j} - f \right). \tag{1.12}$$

We are interested in refining approximations obtained with $T_n := \pi_n T$, where π_n is a sequence of projections with finite rank n. A bounded projection π_n of finite rank n is defined by $\pi_n x := \sum_{j=1}^{n} \langle x\,, e^*_{n,j} \rangle e_{n,j}$ for all $x \in X$, where $(e_{n,j})_{j=1}^n$ is an ordered basis of the range of π_n, and $(e^*_{n,j})_{j=1}^n$ is an adjoint basis of the former in X^*. Hence

$$T_n x := \sum_{j=1}^{n} \langle Tx\,, e^*_{n,j} \rangle e_{n,j}, \quad x \in X. \tag{1.13}$$

We suppose that π_n is pointwise convergent to the identity operator in the Banach X where the operator T is defined. Since T is compact, T_n converges to T in the operator

norm. Let $R(z) := (T - zI)^{-1}$ be the resolvent of T at z. Then $R_n(z) := (T_n - zI)^{-1}$ exists for n large enough and is uniformly bounded, that is, there exists n_0 such that

$$c_0(z) := \sup_{n>n_0} \|R_n(z)\| < +\infty. \tag{1.14}$$

We develop an application in the space $X := L^1([0, \tau_0])$. Let $(\tau_{n,j})_{j=0}^n$ be a grid on $[0, \tau_0]$ such that

$$0 =: \tau_{n,0} < \tau_{n,1} < \cdots < \tau_{n,n-1} < \tau_{n,n} := \tau_0, \tag{1.15}$$

and set

$$h_{n,j} \quad := \quad \tau_{n,j} - \tau_{n,j-1} \quad \text{ for } j \in [1, \dots, n]. \tag{1.16}$$

We define, for $\tau \in [0, \tau_0]$,

$$e_{n,j}(\tau) := \begin{cases} 1 & \text{if } \tau \in (\tau_{n,j-1}, \tau_{n,j}) \\ 0 & \text{otherwise} \end{cases} \tag{1.17}$$

and, for $x \in L^1([0, \tau_0])$,

$$\langle x \, , \, e^*_{n,j} \rangle := \frac{1}{h_{n,j}} \int_{\tau_{n,j-1}}^{\tau_{n,j}} x(\tau') \, d\tau'. \tag{1.18}$$

The product defined in (1.18) is a special case of the scalar product used in equation (1.8) when a grid such as (1.15) is set. In this case the operator in (1.13) is the operator in (1.8) if we choose $\ell_{n,j} = T^\star e^\star_{n,j}$. Let

$$\mu_n := \min\{h_{n,j} \, : \, j \in [1, \dots, n]\}, \quad h_n := \max\{h_{n,j} \, : \, j \in [1, \dots, n]\}, \quad q_n := \frac{\mu_n}{h_n}. \tag{1.19}$$

For quasi-uniform grids, there exists a constant q independent of n such that, for all n, $q \le q_n$. For uniform grids, $q_n = 1$ for all n.

Theorem 2 *Let $\varphi \neq 0$ be the solution of (1.6) with T defined by (1.5). Let φ_n be the solution of (1.9) with T_n defined by (1.8) and (1.15)–(1.17). Then, for n large enough,*

$$\frac{\|\varphi - \varphi_n\|_1}{\|\varphi\|_1} \le \frac{8c_0(z)}{q_n} \int_0^{h_n} g(\tau) \, d\tau, \tag{1.20}$$

where $c_0(z)$ is given by (1.14) and computed with the 1*-norm.*

Proof: See [2]. □

In the case (1.7), the matrix A_n of the linear system (1.10) has entries

$$\mathsf{A}_n(i,j) := \frac{\varpi}{2h_{n,i}} \int_{\tau_{n,i-1}}^{\tau_{n,i}} \int_0^{\tau_0} E_1(|\tau - \tau'|) e_{n,j}(\tau') \, d\tau' \, d\tau, \tag{1.21}$$

and the second member b_n has entries

$$\mathsf{b}_n(i) := \frac{\varpi}{2h_{n,i}} \int_{\tau_{n,i-1}}^{\tau_{n,i}} \int_0^{\tau_0} E_1(|\tau - \tau'|) f(\tau') \, d\tau' \, d\tau. \tag{1.22}$$

For more details, see [3]. An application to the transfer problem in astrophysics gives (1.6) with $z = 1$, and as free term,

$$f(\tau) := \begin{cases} -1 & \text{if } 0 \le \tau \le \tau_0/2, \\ 0 & \text{if } \tau_0/2 < \tau \le \tau_0, \end{cases} \tag{1.23}$$

which describes a sudden drop of the temperature on the $\tau = \tau_0/2$ layer of the atmosphere. For further details on the physical model, see [4].

2 Iterative refinement of approximate solutions

To attain a given precision on the approximate solution φ_n, it may be necessary that the largest grid step h_n be so small that the dimension of the corresponding linear system will be prohibitively large from a computational point of view. Not only the algorithm's stability becomes poor but also the condition number of the matrix may increase if its size increases. Refinement schemes allow us to attain iteratively the exact solution of a large scale linear system by means of the resolution of a sequence of linear systems of moderate fixed size. Let us consider the general framework of a complex Banach space X and a linear compact operator $T : X \to X$. If z is in the resolvent set of T, then $z \neq 0$. Let T_n be a sequence of linear bounded operators in X such that $\|T - T_n\| \to 0$ in the operator norm. Then, for n large enough, z belongs to the resolvent set of T_n and $R_n(z)$ is norm-convergent to $R(z)$.

The most elementary way to refine the approximate solution $\varphi_n := R_n(z)f$ is the following.

$$\text{Scheme A} \quad \begin{cases} x^{(0)} := \varphi_n, \\ x^{(k+1)} := x^{(k)} - R_n(z)(Tx^{(k)} - zx^{(k)} - f), \quad k \ge 0. \end{cases} \tag{2.1}$$

We can interpret $R_n(z)$ as an approximation of the inverse of the Fréchet derivative of the affine operator $x \mapsto (T - zI)x - f$, the exact one being $R(z)$. Since $R(z)$ satisfies the identities

$$R(z) = \frac{1}{z}(R(z)T - I) = \frac{1}{z}(T\,R(z) - I) \tag{2.2}$$

two new different approximations of $R(z)$ are thus motivated,

$$\widetilde{R}_n(z) := \frac{1}{z}(R_n(z)T - I), \quad \widehat{R}_n(z) := \frac{1}{z}(TR_n(z) - I). \tag{2.3}$$

These approximate resolvent operators lead to the following iterative refinement schemes,

$$\text{Scheme B} \quad \begin{cases} \widetilde{x}^{(0)} := \widetilde{R}_n(z)f, \\ \widetilde{x}^{(k+1)} := \widetilde{x}^{(k)} - \widetilde{R}_n(z)(T\widetilde{x}^{(k)} - z\widetilde{x}^{(k)} - f), \quad k \ge 0, \end{cases} \tag{2.4}$$

$$\text{Scheme C} \quad \begin{cases} \widehat{x}^{(0)} := \widehat{R}_n(z)f, \\ \widehat{x}^{(k+1)} := \widehat{x}^{(k)} - \widehat{R}_n(z)(T\widehat{x}^{(k)} - z\widehat{x}^{(k)} - f), \quad k \ge 0. \end{cases} \tag{2.5}$$

Since the computation of residuals which tend to zero, as well as the resolution of almost homogeneous linear systems may be unstable, the following theorems are interesting for algorithmic purposes.

Theorem 3 *In (2.1),* $x^{(k+1)} = x^{(0)} + R_n(z)(T_n - T)x^{(k)}$ *for* $k \geq 0$.

Theorem 4 *In (2.4),* $\widetilde{x}^{(k+1)} = \widetilde{x}^{(0)} + \frac{1}{z}R_n(z)(T_n - T)T\widetilde{x}^{(k)}$ *for* $k \geq 0$.

Theorem 5 *In (2.5),* $\widehat{x}^{(k+1)} = \widehat{x}^{(0)} + \frac{1}{z}TR_n(z)(T_n - T)\widehat{x}^{(k)}$ *for* $k \geq 0$.

Proof: For each $k \geq 0$, in (3),

$$\begin{aligned} x^{(k+1)} &= x^{(k)} - R_n(z)(Tx^{(k)} - zx^{(k)} - f) \\ &= x^{(k)} - R_n(z)(T - T_n + T_n - zI)x^{(k)} + x^{(0)} \\ &= x^{(0)} + R_n(z)(T_n - T)x^{(k)} \end{aligned}$$

For (4) and (5), the proof follows the same idea but it is technically more complicated. □

In our application to the transfer equation in astrophysics, T is defined by (1.5) with g given by (1.7), and the equation (1.6) has $z = 1$.

3 Numerical computations

The iterative refinement schemes allow us to obtain the exact solution of a large scale linear system by solving a sequence of moderate fixed size ones. Each of the three iterative refinement schemes presented in this work are based on an approximation, say $G_n(z)$, of the resolvent operator $R(z)$. Their common structure is the following.

$$\left\{ \begin{array}{rcl} \xi^{(0)} &:=& G_n(z)f, \\ \xi^{(k+1)} &:=& \xi^{(0)} + (I - G_n(z)(T - zI))\xi^{(k)}, \quad k \geq 0. \end{array} \right. \tag{3.1}$$

Theorem 6 *Let* $c_1(z) := 8c_0(z)\max\{1, \|T\|_1/|z|\}$, *and* $(\xi^{(k)})_{k\geq 0}$ *be any of the sequences (2.1), (2.4) or (2.5). Then*

$$\frac{\|\xi^{(k)} - \varphi\|_1}{\|\varphi\|_1} \leq \left(\frac{c_1(z)}{q_n}\int_0^{h_n} g(\tau)\,d\tau\right)^{k+1}, \quad k \geq 0.$$

Proof: Let us prove the bound for the sequence defined by (2.1). For the other two, the arguments are similar. Using Theorem 3, we have

$$\begin{aligned} x^{(k)} - \varphi &= \left(R_n(z)(T_n - T)\right)^k (x^{(0)} - \varphi), \\ x^{(0)} - \varphi &= R_n(z)(T - T_n)\varphi. \end{aligned}$$

Hence,

$$\|x^{(k)} - \varphi\|_1 \leq \|(R_n(z)(T - T_n))^{k+1}\|_1 \|\varphi\|_1,$$

and, in [2], we have shown that $\|R_n(z)(T_n - T)\|_1 \leq \dfrac{8c_0(z)}{q_n}\displaystyle\int_0^{h_n} g(\tau)\,d\tau$. □

All the schemes need evaluations of T at some prescribed functions of X. In practice T is not used for this purpose but an operator T_m of the sequence $(T_\nu)_{\nu\geq 1}$ is used instead,

where $m > n$. We consider the kernel g defined by (1.7) and the free term f defined by (1.23). Table 1 gives the number of iterations performed by each scheme for several values of ϖ in order to obtain a first relative residual less than or equal to 10^{-12}, when a quasi-uniform grid $(\tau_{\nu,i})_{i=0}^{\nu}$ is built such that ν is a multiple of 10, $\tau_0 = 1000$,

$$n = 200, \quad m = 1000, \quad \text{and} \quad h_{\nu,i} := \begin{cases} \dfrac{\tau_0}{2\nu} & \text{if} \quad i \in [1, \ldots, \frac{\nu}{5}], \\[2ex] \dfrac{\tau_0}{5\nu} & \text{if} \quad i \in [\frac{\nu}{5}+1, \ldots, \frac{\nu}{2}], \\[2ex] \dfrac{\tau_0}{2\nu} & \text{if} \quad i \in [\frac{\nu}{2}+1, \ldots, \frac{9\nu}{10}], \\[2ex] \dfrac{4\tau_0}{\nu} & \text{if} \quad i \in [\frac{9\nu}{10}+1, \ldots, \nu]. \end{cases} \tag{3.2}$$

Albedo ϖ	Scheme A (2.1)	Scheme B (2.4)	Scheme C (2.5)
0.750	29	15	14
0.990	46	27	26
0.999	385	196	195

TAB 1. Number of iterations.

Figures 1, 2 and 3 show the last iterate of all schemes, as well as the corresponding convergence histories, for $\varpi \in \{0.750, 0.990, 0.999\}$. As we can see, the schemes B and C are much faster than Atkinson's formula A, specially when the albedo is close to 1. In the latter situation a wider boundary layer arises at the left of the atmosphere, and the decay at the middle point takes place along a wider subinterval.

A survey on different discretization methods for integral operators can be found in [1], with special emphasis on spectral applications. In what concerns condition number of associated linear systems, the reader is refered to [7], [5] and [6].

Bibliography

1. M. Ahues, A. Largillier and B.V. Limaye, *Spectral Computations with Bounded Operators*, Chapman and Hall, Boca Raton, 2001.
2. M. Ahues, A. Largillier and O. Titaud, The roles of a weak singularity and the grid uniformity in the relative error bounds, Numer. Funct. Anal. and Optimiz. **22**, 789–814, 2001.
3. M. Ahues, F. D'Almeida, A. Largillier, O. Titaud and P. Vasconcelos, An L^1 Refined Projection approximate solution of the radiation transfer equation in stellar atmospheres, Journal of Computational and Applied Mathematics **140**, 13–26, 2002.
4. I. W. Busbridge, *The Mathematics of Radiative Transfer*, Cambridge University Press, 1960.

5. L. N. Desphande and B.V. Limaye, On the stability of singular finite-rank methods, SIAM J. Numer. Anal. **27**, 792–803, 1990.
6. A. Largillier and B.V. Limaye, Finite-rank methods and their stability for coupled systems of operator equations, SIAM J. Numer. Anal. **2**, 707–728, 1996.
7. R. Whitley, The stability of finite-rank methods with applications to integral equations, SIAM J. Numer. Anal. **23**, 118–134, 1986.

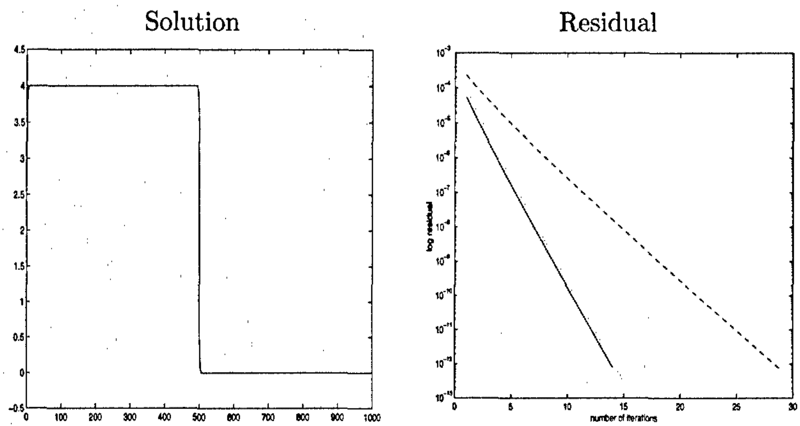

FIG. 1. Solution and convergence history for $\varpi = 0.750$: Scheme A — dashed line, Scheme B — dotted line, Scheme C — solid line.

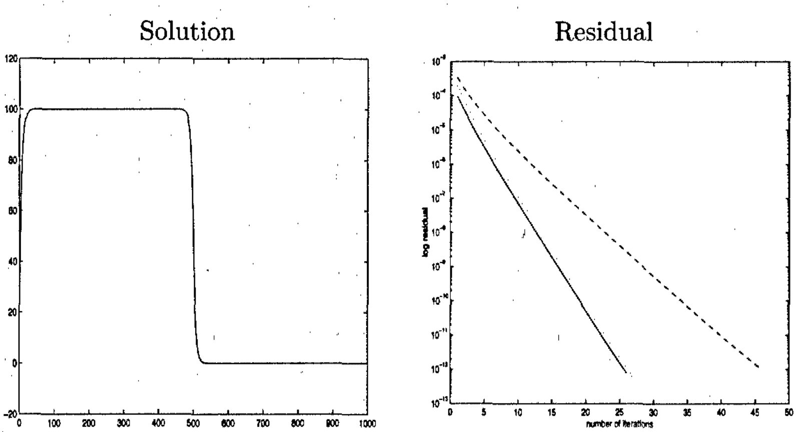

FIG. 2. Solution and convergence history for $\varpi = 0.990$: Scheme A — dashed line, Scheme B — dotted line, Scheme C — solid line.

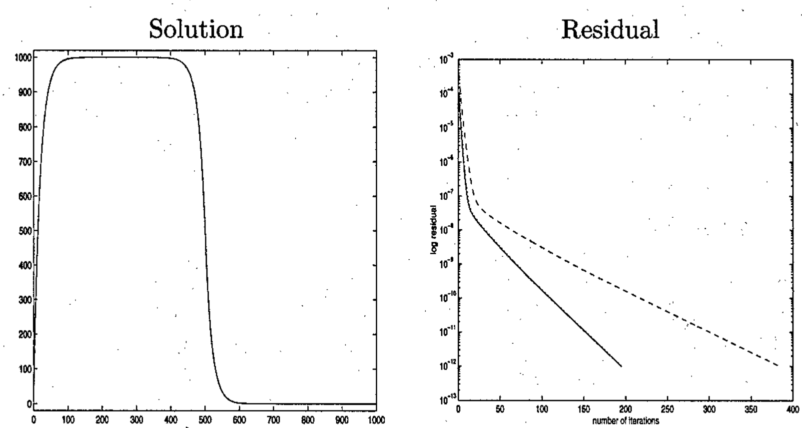

FIG. 3. Solution and convergence history for $\varpi = 0.999$: Scheme A — dashed line, Scheme B — dotted line, Scheme C — solid line.